

Grazing incidence fast atom diffraction for He atoms impinging on a Ag(110) surface

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Abstract

Experimental diffraction patterns produced by grazing scattering of fast helium atoms from a Ag(110) surface are used as a sensitive tool to test both the scattering and the potential models. To describe the elastic collision process we employ the surface eikonal (SE) approximation, which is a semi-classical method that includes the quantum interference between contributions coming from different projectile paths. The projectile-surface potential is derived from an accurate density-functional theory (DFT) calculation that takes into account the three degrees of freedom of the incident projectile. A fairly good agreement between theoretical and experimental momentum distributions is found for incidence along different low-indexed crystallographic directions.

I. INTRODUCTION

Since the unexpected observation of grazing incidence diffraction of fast atoms (GIFAD) on crystal surfaces [1, 2], extensive research, both experimental and theoretical, has been devoted to the subject [3–10]. The first experimental evidences of this phenomenon were reported at insulator materials [1, 2], where the presence of a wide band-gap helps to suppress inelastic processes, thus preventing quantum decoherence [11]. Soon afterwards the effect was observed at semi-conductor [12] and metallic surfaces [7, 13] even though, in the case of metals, energy loss values were found to be significant [7, 14, 15]. In addition, GIFAD patterns have displayed an exceptional sensitivity to the projectile-surface interaction, making it possible to study very subtle contributions, like the ones produced by surface rumpling [5, 16, 17] or by adsorbed structures [18, 19]. Nowadays GIFAD is becoming a promissory tool for examining the electronic and morphological characteristics of solid-vacuum interfaces [12, 20–22].

The aim of this work is to investigate the diffraction patterns produced by fast He atoms grazingly impinging on a Ag(110) surface. Since this collision system corresponds to the first and simplest metallic case for which GIFAD effects were experimentally observed [7], it provides a useful prototype to test both the theoretical method and the surface potential model. To describe the scattering process we employ a distorted wave theory – the surface eikonal (SE) approximation – that makes use of the eikonal wave function to represent the elastic collision with the surface, while the projectile motion is classically described using different initial conditions [6]. The SE approach has been used to evaluate GIFAD distributions from insulator surfaces, providing results in good agreement with the experimental data [23–25]. It has also been applied to the elastic scattering of fast N atoms from a (111) silver surface, for which asymmetries in the diffraction patterns might be originated by second atomic layer effects in the surface potential [26].

Due to the strong dependence of the interference patterns on the atom-surface interaction, a crucial issue of the theoretical description is the detailed representation of the projectile-surface potential. In Refs. [7, 14] the He-Ag(110) potential was simulated as a two-dimensional sinusoidal function, whose corrugation amplitude was derived from experimental data by means of the Hard-Wall approximation. Here we use a potential energy surface (PES) that was built from a large set of *ab initio* data obtained with the DFT-based

“QUANTUM ESPRESSO” code [27], combined with a sophisticated interpolation technique [28]. From such *ab initio* values we derived a three-dimensional (3D) PES, taking into account the projectile’s three degrees of freedom. No average of the surface potential along the incidence direction was considered in the calculation.

In this article, eikonal projectile distributions derived by using the DFT potential are compared with experimental data for three different incidence directions: $[1\bar{1}0]$, $[001]$, and $[1\bar{1}2]$. The paper is organized as follows. The theoretical method, including details of the potential calculation, is summarized in Sec. II, results are presented and discussed in Sec. III, and in Sec. IV we outline our conclusions. Atomic units (a.u.) are used unless otherwise stated.

II. THEORETICAL MODEL

A. The transition amplitude

Within the SE approximation, the scattering state of the projectile is represented with the eikonal wave function [6],

$$\Psi_i^+(\vec{R}_P, t) = \phi_i(\vec{R}_P) \exp(-i\eta(t)), \quad (1)$$

where \vec{R}_P is the position vector of the incident atom, $\phi_i(\vec{R}_P) = (2\pi)^{-3/2} \exp(i\vec{K}_i \cdot \vec{R}_P)$ is the initial unperturbed wave function, with \vec{K}_i the initial projectile momentum, and the sign $+$ indicates the outgoing asymptotic conditions. In Eq. (1) the function $\eta(t)$ denotes the eikonal-Maslov phase, which depends on the classical position of the projectile at the time t , $\vec{R}_P(t)$, as [24]:

$$\eta(t) = \int_{-\infty}^t dt' V_{SP}(\vec{R}_P(t')) + \phi_M, \quad (2)$$

where V_{SP} is the projectile-surface interaction and $\phi_M = \nu\pi/2$ is the Maslov correction that takes into account the phase change of the scattering wave function as it passes through a focus, with the Maslov index ν defined as in Ref. [29].

By introducing Eq. (1) in the usual definition of the T-matrix element [30], the SE transition matrix per unit area \mathcal{A} reads [24].

$$T_{if}^{(SE)} = \frac{1}{\mathcal{A}} \int_{\mathcal{A}} d\vec{R}_{os} a_{if}(\vec{R}_{os}), \quad (3)$$

where \vec{R}_{os} is the initial position of the projectile on the surface plane and

$$a_{if}(\vec{R}_{os}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{+\infty} dt |v_z(\vec{\mathcal{R}}_P)| V_{SP}(\vec{\mathcal{R}}_P) \times \exp[-i\vec{Q} \cdot \vec{\mathcal{R}}_P - i\eta(t)] \quad (4)$$

is the transition amplitude associated with the classical path $\vec{\mathcal{R}}_P = \vec{\mathcal{R}}_P(\vec{R}_{os}, t)$. The vector $\vec{Q} = \vec{K}_f - \vec{K}_i$ is the momentum transfer, with the final projectile momentum \vec{K}_f verifying energy conservation, i.e. $|\vec{K}_f| = |\vec{K}_i|$. The function $v_z(\vec{\mathcal{R}}_P)$ represents the component of the projectile velocity that is perpendicular to the surface plane, with \hat{z} along the surface normal, aiming towards the vacuum region.

From Eq. (3), the differential probability, per unit of surface area, for elastic scattering with final momentum \vec{K}_f in the direction of the solid angle $\Omega_f \equiv (\theta_f, \varphi_f)$ is $dP^{(SE)}/d\Omega_f = (2\pi)^4 m_P^2 |T_{if}^{(SE)}|^2$, where m_P is the projectile mass, and θ_f and φ_f are the final polar and azimuthal angles, respectively, with φ_f measured with respect to the incidence direction in the surface plane. Details are given in Refs. [6, 24].

B. Projectile-surface interaction

The interaction energy of the He atom with the Ag(110) surface is described with a full adiabatic 3D PES that depends on the atomic position $\vec{R}_P = (X, Y, Z)$. The PES is constructed from a grid of *ab initio* energies for 42 Z values and 6 (XY) sites, chosen as indicated in Fig. 1, over which an interpolation is performed [28].

All *ab initio* data are obtained from the DFT-based “QUANTUM ESPRESSO” code [27]. The values of relevant input parameters are chosen so that *ab initio* energies are calculated to a prescribed accuracy (differences < 5 meV with respect to the converged result). The exchange-correlation energy is calculated within the generalized gradient approximation (GGA), using the Perdew-Burke-Ernzerhof energy functional (PBE) [31]. The electron-core interaction is described with ultra-soft pseudopotentials [32]. The energy cutoff in the plane-wave expansion is 35.0 Ryd for the wave functions and 245.0 Ryd for the charge density and potential; the fractional occupancies are determined through the broadening approach of Marzari-Vanderbilt [33] with $\sigma = 0.01$ Ryd.; and the Brillouin-zone integration is performed

with a $10 \times 7 \times 1$ Monkhorst-Pack Grid of special k points. The Ag lattice constant is $a = 7.865$ a.u.

The Ag(110) surface is modeled by means of the supercell-slab scheme. A four-layer slab is used with a 2×2 cell in the plane parallel to the surface and a supercell of length 25.03 a.u. along the normal to the surface (\hat{z} axis). The energy for He-Ag(110) with the He atom midway between slabs provides a reasonable representation of the asymptotic region and is chosen as the energy reference. The surface interlayer distance is relaxed from its bulk value $d_0 = 2.781$ a.u., keeping the two bottom layers fixed. Geometry corrections due to relaxation amount to -9.14% and +4.11% for the first and second interlayer distances respectively, in accord with experimental results [34]. Once relaxed, the slab is kept frozen for the calculations that follow.

Given the closed-shell electronic structure of the He atom ($1s^2$), we perform a non spin-polarized calculation of the ground state. A quality check of the interpolation shows that the error introduced is < 1 meV, well below the prescribed accuracy for the *ab initio* data. In Figs. 2 a) and b) we show the equipotential curves along the directions $[001]$ and $[1\bar{1}0]$, respectively, both starting from a site corresponding to an atom of the first layer.

III. RESULTS

In this work we use the SE approximation to study momentum distributions of ^3He atoms elastically scattered from a Ag(110) surface under grazing incidence conditions. Within the SE approach the perpendicular momentum distribution is derived from the double differential probability $dP^{(SE)}/d\Omega_f$ as

$$\frac{dP^{(SE)}}{dQ_{\text{tr}}} = \int d\theta_f \frac{\cos \theta_f}{\sqrt{K_{fs}^2 - Q_{\text{tr}}^2}} \frac{dP^{(SE)}}{d\Omega_f}, \quad (5)$$

where $K_{fs} = K_f \cos \theta_f$ is the final momentum parallel to the surface and $Q_{\text{tr}} = K_f \cos \theta_f \sin \varphi_f$ is the component of the momentum transfer in the transverse direction, which is perpendicular to the incidence direction on the surface plane.

Like in Refs. [7, 14], projectile impact along three different channels of the silver surface - $[1\bar{1}0]$, $[001]$, and $[1\bar{1}2]$ - is considered (see Fig. 1). Note that in contrast with the notation employed in Refs. [7, 14], here the figures will be labeled with the direction of the incident

beam, rather than with the probed direction, which is perpendicular to \vec{K}_i . For each of these directions, we evaluated $T_{if}^{(SE)}$ from Eq. (3) using 4×10^5 classical trajectories with random initial positions \vec{R}_{os} that vary within an area \mathcal{A} . In this work, in order to resemble the incident wave packet we use Gaussian distributions along the incidence and transverse directions, with full widths at half maximum determined by the size of \mathcal{A} , to evaluate the random initial positions of projectile trajectories [30, 35]. For an almost perfect plane-wave beam, the area \mathcal{A} is large and includes several reduced unit cells.

In Fig. 3 we compare theoretical and experimental perpendicular momentum spectra for He atoms impinging along the $[1\bar{1}0]$ direction. The incidence energy is $E_i = K_i^2/(2m_P) = 500$ eV and the polar incidence angle, measured with respect to the surface plane, is $\theta_i = 0.75^\circ$. It corresponds to a perpendicular energy, associated with the movement normal to the surface, $E_{i\perp} = E_i \sin^2 \theta_i = 86$ meV. Under this incidence condition, the experimental momentum distribution presents a rich diffraction pattern, with maxima and minima almost symmetrically placed with respect to the incidence direction, for which $Q_{tr} = 0$. For a detailed analysis of this spectrum, SE differential momentum probabilities, obtained by considering in Eq. (3) an integration region \mathcal{A} equal to 8×8 reduced unit cells, are displayed in the figure with a blue dashed line. These results present narrow Bragg maxima placed at $Q_{tr} = m2\pi/d$, with m an integer number and d the distance between parallel atomic rows along the incidence channel, whose positions coincide with those of the experimental maxima. Within the SE approach, the width of these Bragg peaks is governed by the number of reduced unit cells along the perpendicular direction, n_{tr} (in our case, $n_{tr} = 8$), decreasing as n_{tr} increases, while their intensities are determined by the supernumerary rainbow distribution, as explained below.

The two different mechanisms - Bragg diffraction and supernumerary rainbows - that are present in GIFAD patterns [3] can be analyzed separately with the SE model. The SE transition matrix can be factorized as [25]

$$T_{if}^{(SE)} = \tilde{T}_1^{(SE)} S_{n_{tr}}(Q_{tr}), \quad (6)$$

where $\tilde{T}_1^{(SE)}$ is derived from Eq. (3) by evaluating the \vec{R}_{os} -integral over *one* reduced unit cell, and $S_{n_{tr}}(Q_{tr}) = \sin(n_{tr} \beta)/(n_{tr} \sin \beta)$, with $\beta = Q_{tr}d/2$, for incidence along the $[1\bar{1}0]$ and $[001]$ directions. The factor $\tilde{T}_1^{(SE)}$, associated with supernumerary rainbows, is produced by interference between projectile trajectories whose initial positions are separated by a

distance smaller than d . In turn, $S_{n_{\text{tr}}}(Q_{\text{tr}})$, which gives rise to the Bragg peaks, is due to interference between projectile trajectories whose initial positions are separated by a distance just equal to a multiple of d . The positions of Bragg peaks, indicated with vertical dashed lines in Figs. 3 and 4, provide information about the crystallographic structure only, but their intensities, which are modulated by the supernumerary rainbow factor $\tilde{T}_1^{(SE)}$, depend strongly on the shape of the PES across the incidence channel. In fact, the factor $\tilde{T}_1^{(SE)}$ completely determines the number and the intensity of observed Bragg maxima, even suppressing them, as approximately happens for the Bragg peaks of order $m = \pm 1$ in Fig. 3.

In order to compare with the experimental data, in Fig. 3 we also plot SE differential probabilities convoluted with a Lorentz function (red solid line) to simulate the experimental conditions. The parameters of the line broadening are taken from the observed linewidths, as stated in Ref. [7]. Such a convolution takes into account not only the experimental divergence of the incident beam but also the broadening introduced by both thermal vibrations of lattice atoms and inelastic processes, which contribute to spoil the coherence [36]. We found a good agreement between the convoluted SE results and the experiment in the whole range of perpendicular momenta, with the exception of the maxima of order $m = \pm 3$ whose intensity is overestimated by the SE curve. This fact is related to the sharpness of the rainbow peaks of the envelope function $\tilde{T}_1^{(SE)}$, which is originated by the classical description of the projectile motion that does not include the finite intensity on the dark side of the classical rainbow [37]. Such classical rainbow maxima affect the intensity of the outermost Bragg peaks of the GIFAD pattern only when they are close to each other, as observed in the figure. However, this deficiency does not influence the SE distribution at smaller transverse momenta.

The final perpendicular momentum distribution of a He beam impinging along a less corrugated crystallographic channel - the [001] channel - is shown in Fig. 4 for the incidence parameters $E_i = 500$ eV and $\theta_i = 1.0^\circ$ (i.e., a perpendicular energy $E_{i\perp} = 180$ meV). Here, SE results obtained by considering initial positions inside $n_{\text{tr}} = 16$ unit cells are plotted in the figure together with the convoluted values. The SE momentum spectrum, including experimental and inherent uncertainties through convolution, is in fairly good accord with the experimental data. Notice that the Q_{tr} position of the classical rainbow peak depends on $E_{i\perp}$, and for this incidence condition it is again close to the outermost Bragg maximum.

On the other hand, the number of observed Bragg maxima is determined by $\tilde{T}_1^{(SE)}$, being sensitive to the potential contour across the incidence direction. Then, as a consequence of the much lower corrugation of the channel, observed in Fig. 2, the projectile momentum spectrum is narrower than the one of Fig. 3.

Finally, in Fig. 5 we compare experimental and theoretical diffraction charts for 1 keV ^3He atoms impinging on the silver surface along the $[1\bar{1}2]$ channel. These diffraction charts display the intensity of the projectile distribution as a function of the transverse transferred momentum and the incidence angle θ_i (or the normal impact energy), providing an overall scenery of the GIFAD patterns for this low-indexed crystallographic direction. The experimental diffraction chart of Fig. 5 (a) was obtained by considering intensity distributions corresponding to 38 different incidence angles. Like in Fig. 4, as a consequence of the low corrugation of the channel, only three diffraction orders - $m = 0$ and $m = \pm 1$ - are visible in the figure. However, since the number of observed Bragg maxima depends strongly on the shape of the equipotential curves across the incidence channel [5], and different values of $E_{i\perp}$ allow one to probe such potential contours for different distances to the surface, the general agreement between the experimental and simulated two-dimensional diffraction charts of Fig. 5 is a signature of the quality of the present DFT potential in the 0.10 - 0.45 eV range of perpendicular energies.

IV. CONCLUSIONS

GIFAD patterns for helium atoms colliding with a silver surface are used to test both the SE approach and the *ab initio* DFT surface potential, for the case of a metal target. The SE approximation takes into account the quantum interference produced by the coherent superposition of transition amplitudes for different projectile paths that end with the same final momentum, while the *ab initio* potential was obtained from DFT by making use of the “QUANTUM ESPRESSO” code.

For the He-Ag(110) system, experimental momentum spectra along different crystallographic directions display defined interference structures that are fairly well reproduced by the theoretical results. Taking into account the extreme sensitivity of fast atom diffraction patterns, this agreement between SE differential momentum probabilities and experimental data is indicative of the proper description of the atom-surface interaction given by the DFT

potential. Further experimental and theoretical research has been recently carried out in order to make a deeper examination of the potential model, considering a wider normal energy range [38].

Acknowledgments

C.R.R and M.S.G. acknowledge financial support from CONICET, UBA, and ANPCyT of Argentina. One of us (M.S.G) would like to express gratitude to the Université Paris-Sud for support during a portion of this work. G.A.B. acknowledges financial support by ANPCyT and is also thankful to Dr. H.F. Busnengo, Dr. J.D. Führ and Dr. M.L. Martiarena regarding the PES calculation. The experimental work was supported by the ANR under contract number ANR-07-BLAN-0160-01.

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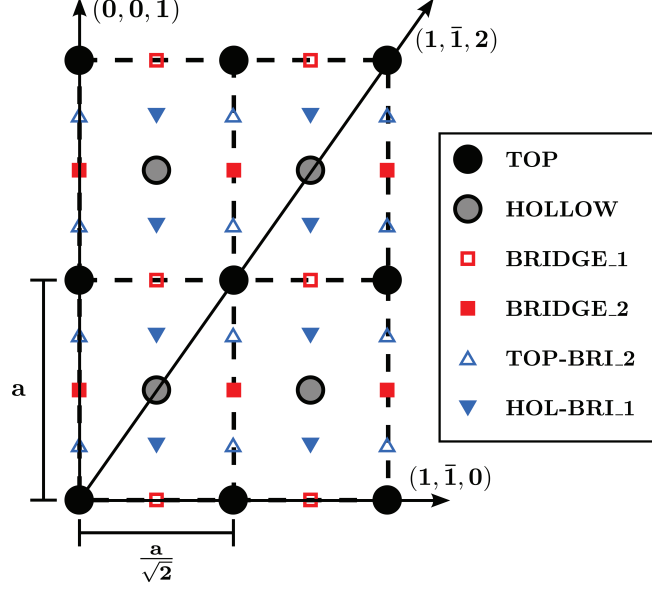


FIG. 1: (Color online) Geometry of the Ag(110) surface. a is the lattice constant. The six (XY) sites shown in the figure correspond to the ones used for the PES calculation. Circles, TOP and HOLLOW sites standing for atoms of the first and second layers, respectively; squares, BRIDGE_1 and BRIDGE_2 sites corresponding to the middle points between first and second TOP atomic neighbors, respectively; triangles, middle points between the mentioned sites. The incidence directions of He atoms are also indicated.

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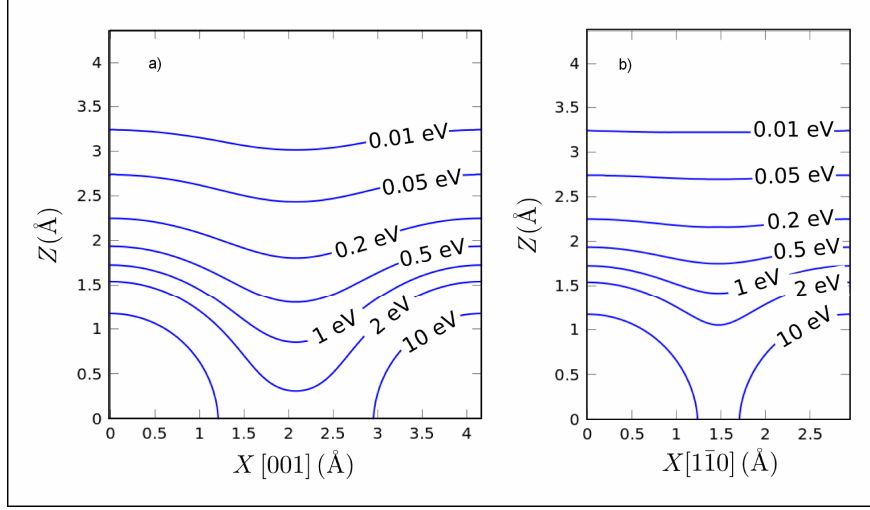


FIG. 2: (Color online) Distances Z to the surface plane (topmost atomic layer) of equipotential curves for the interaction between the He atom and the Ag(110) surface. The value $X=0$ corresponds to a TOP site, as indicated in Fig. 1. a) Equipotential curves as a function of the coordinate along the $[001]$ direction, $X[001]$, for $X[1\bar{1}0] = 0$; b) similar to a) as a function of the coordinate along the $[1\bar{1}0]$ direction, $X[1\bar{1}0]$, for $X[001] = 0$.

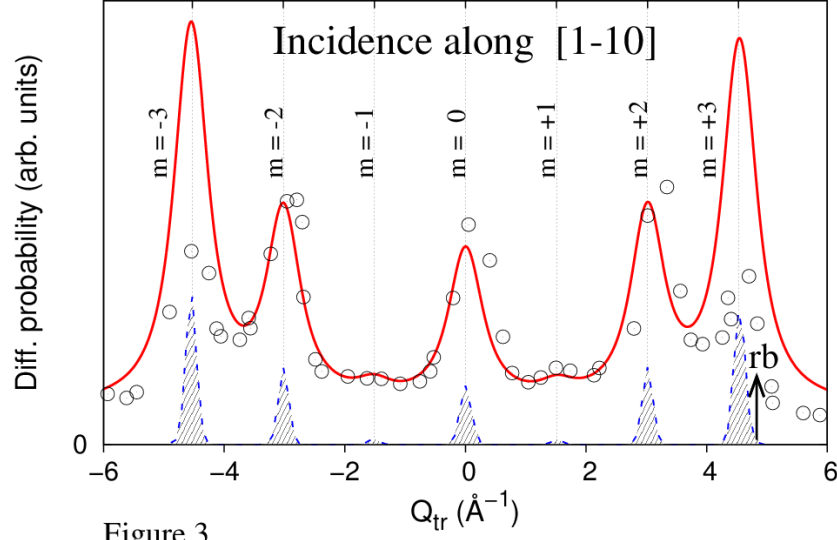


Figure 3

FIG. 3: (Color online) Momentum distribution, as a function of the perpendicular momentum transfer Q_{tr} , for ^3He atoms impinging on Ag(110) surface along the $[1\bar{1}0]$ direction. The incidence energy and angle are $E_i = 500$ eV and $\theta_i = 0.75^\circ$, respectively. Solid red line, SE differential momentum probability convoluted to include uncertainties as explained in the text [36]; dashed blue line, SE differential momentum probability for $n_{\text{tr}} = 8$ (without convolution); empty circles, experimental data from Ref. [7]. The vertical dashed lines show Bragg peak positions and the arrow indicates the position of the classical rainbow maximum.

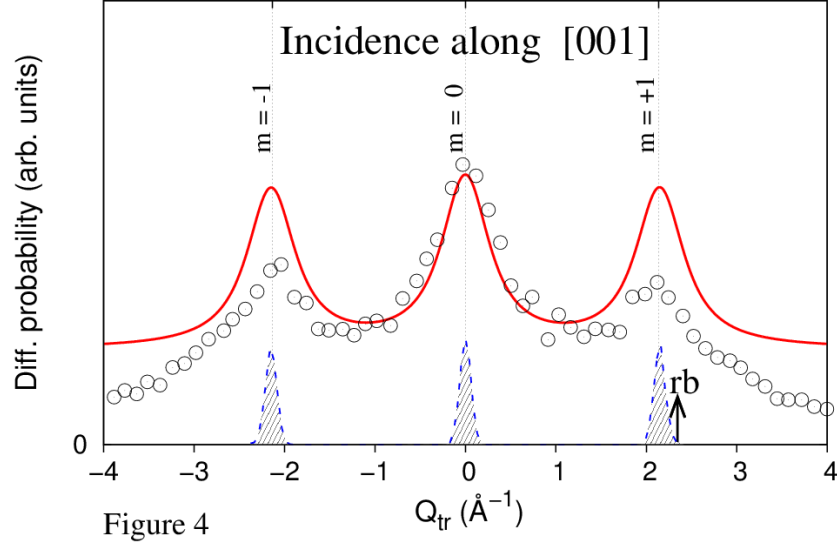


FIG. 4: Similar to Fig. 3 for ${}^3\text{He}$ atoms impinging along the $[001]$ direction with $E_i = 500$ eV and $\theta_i = 1.0^\circ$. Empty circles, experimental data extracted from Ref. [15].

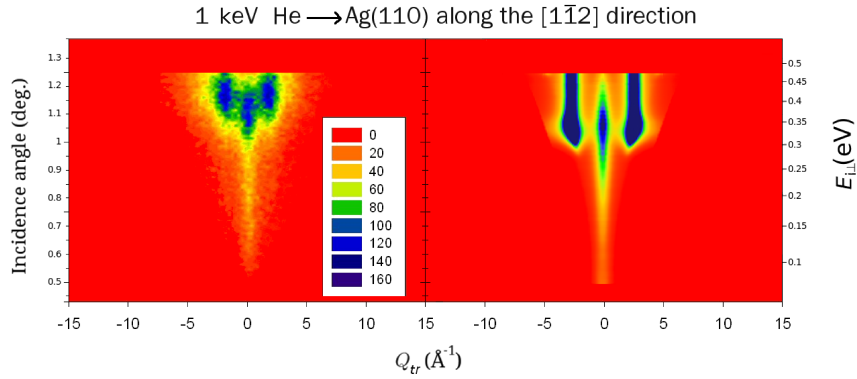


FIG. 5: (Color online) Two-dimensional diffraction chart displaying (a) experimental intensities and (b) SE differential momentum probabilities, as a function of the transverse momentum transfer Q_{tr} and the incidence angle θ_i (or the normal energy $E_{i\perp}$), for 1 keV ${}^3\text{He}$ atoms impinging along the $[1\bar{1}2]$ direction.